# Universality in Heavy Fermions Revisited

Mucio A.Continentino

Instituto de Fisica, Universidade Federal Fluminense Campus da Praia Vermelha, Niterói, 24.210-340, RJ, Brasil (February 1, 2008)

A previous scaling analysis of pressure experiments in heavy fermion is reviewed and enlarged. We show that the critical exponents obtained from this analysis indicate that a one-parameter scaling describes these experiments. We obtain explicitly the enhancemente factors showing that these systems are indeed near criticality and that the scaling approach is appropriate. The physics responsible for the one-parameter scaling and breakdown of hyperscaling is clarified. We discuss a microsocopic theory that is in agreement with the experiments. The scaling theory is generalized for the case the *shift* and *crossover* exponents are different. The exponents governing the physical behavior along the non-Fermi liquid trajectory are obtained for this case.

PACS Nos. 71.27+a 75.30Mb 71.10Hf 75.45+j 64.60Kw

### I. INTRODUCTION

The scaling theory of heavy fermions is based on the existence of a quantum critical point (QCP) which governs the physical behavior of these systems [2–5]. It yields the following scaling relations for the singular part of the free energy density

$$f \propto |\delta|^{2-\alpha} F\left[\frac{T}{T_{coh}}, \frac{H}{|\delta|^{\beta+\gamma}}, \frac{h}{h_c}\right]$$
 (1)

where the coherence temperature,  $T_{coh} = |\delta|^{\nu z}$  and the characteristic uniform field,  $h_c = |\delta|^{\phi_h}$ . H and h are staggered and uniform magnetic fields respectively. The scaling properties of relevant thermodynamic quantities, like the uniform susceptibility,  $\chi_0 \propto \partial^2 f/\partial h^2$ , the thermal mass,  $m_T = C/T \propto \partial^2 f/\partial T^2$ , for  $T \ll T_{coh}$  are obtained from Eq.1. The critical exponents obey standard scaling relations but hyperscaling is modified due to the quantum character of the critical point. It is given by  $2 - \alpha = \nu(d+z)$  where z is the dynamic exponent and d the dimension of the system [3]. The quantity  $\delta = (J/W) - (J/W)_c$  measures the distance to the QCP. J and W are parameters of the Kondo lattice Hamiltonian, the coupling between localized and conduction electrons and the bandwidth, respectively.

## II. SCALING ANALYSIS

In heavy fermions the ratio (J/W) depends on volume V and consequently on pressure P. Let us define the critical volume  $V_c$  as the volume at which  $(J/W) = (J/W)_c$ . Consider a physical quantity which close to  $V_c$  behaves as  $X(P) = A|(V - V_c)/V_c|^{-x}$  where V is the volume at pressure P. If we introduce a reference pressure  $P_0$  (volume  $V_0$ ) we have:

$$\frac{X(P)}{X(P_0)} = \left(\frac{V - V_c}{V_0 - V_c}\right)^{-x} = \left(\frac{V - V_0 + V_0 - V_c}{V_0 - V_c}\right)^{-x}$$
(2)

Defining,  $\delta_0 = V_0 - V_c$  and  $\Delta V = V - V_0$ , where the latter gives the change in volume due to the pressure change  $\Delta P = P - P_0$ , we get

$$\frac{X(P)}{X(P_0)} = \left(\frac{\Delta V + \delta_0}{\delta_0}\right)^{-x} = \left(1 + \frac{\Delta V}{\delta_0}\right)^{-x} \tag{3}$$

Then

$$Ln\left[\frac{X(P)}{X(P_0)}\right] = -xLn\left(1 + \frac{\Delta V}{\delta_0}\right) \tag{4}$$

For  $\Delta V$  sufficiently small, or small changes of pressure from the reference pressure, we have  $\Delta V = -\kappa_0 V_0 \Delta P$  where the compressibility is given by  $\kappa_0 = (-1/V)(\partial V/\partial P)$ . In the limit that  $(\Delta V/\delta_0) \ll 1$  we obtain

$$Ln\left[\frac{X(P)}{X(P_0)}\right] \approx x\kappa_0(V_0/\delta_0)\Delta P$$
 (5)

where  $(V_0/\delta_0) = V_0/(V_0 - V_c) = \alpha_V/(\alpha_V - 1)$  with  $\alpha_V =$  $V_0/V_c$ . The equation above holds if the system at the reference pressure  $P_0$  is not too close to the quantum critical point, otherwise the condition  $(\Delta V/\delta_0) \ll 1$ , or equivalently  $(\kappa_0 \Delta P \alpha_V)/(1-\alpha_V) \ll 1$  is not satisfied. Note that in Eq.5 the coefficient of  $\Delta P$  depends on the critical exponent x associated with the physical quantity X. The validity of Eq. 5 for several physical quantities at and below the coherence line has been verified for the heavy fermions  $CeRu_2Si_2$ ,  $CeAl_3$ ,  $UPt_3$  and  $CeCu_6$  as shown in Fig.1 [3]. These materials are located in the non-critical side  $(V < V_c)$  of Doniach's phase diagram. For  $CeAl_3$  a reference pressure of 1.2 kbars has been used to guarantee that this is the case, otherwise  $P_0 = 0$ . The collapse of the different data for a given material on a single line, as shown in Fig.1, implies the following relations among the critical exponents [3],  $2 - \alpha = \nu z$ and  $\phi_h = \nu z$ . The meaning and implications of these relations will be discussed further down. The inclination of the lines in Fig. 1, i.e.,  $\Gamma_V = Ln \left[ \frac{X(P)}{X(P_0)} \right] / \Delta P$ , for different compounds are given in Table 1. From Eq.5

we note that the Grüneisen parameters  $\Omega_V = (\Gamma_V/\kappa_0) = x\alpha_V/(\alpha_V-1)$  provide essentially the enhancement factors due to the proximity of the quantum phase transition. Assuming, for example, that x=-1 as we will discuss below, the results for  $\Omega_V$  in Table 1 yield values of  $\alpha_V$  ranging from  $\alpha_V \approx 0.97$  to  $\alpha_V \approx 0.99$  as shown in this Table. This clearly indicates that the systems we are considering are close to the QCP and a scaling analysis is justified.

Consider the case of  $CeCu_6$ . Eq.1 yields,  $m_T = C/T \propto \partial^2 f/\partial T^2 \propto |\delta|^{2-\alpha-2\nu z}$ . From the experimental relation  $2-\alpha = \nu z$ , we get  $m_T^{-1} \propto |(V_0 - V_c)/V_c|^{\nu z} = (1-\alpha_V)^{\nu z}$ . Taking x = -1, i.e.,  $\nu z = 1$ , as before (see also below), we get an enhancement factor  $\Omega_V/\alpha_V = 1/(1-\alpha_V)$  for the thermal mass,  $m_T$ , of this material of approximately 120.

The data in Table 1 calls attention to the fact that  $\Omega_V$  is larger for  $CeRu_2Si_2$ , although this system has the smallest thermal mass of the four compounds [6]. In order to conciliate this result with the idea of universality, i.e., that the critical exponents are the same for a given quantity independent of the material, it is important to write the enhancement factor in terms of the parameters of the Kondo lattice Hamiltonian. For this purpose we need a relation between (J/W) and the volume. We assume that  $j(V)=(J/W)=(J/W)_0exp(-q(\frac{V-V_0}{V_0}))$  where  $(J/W)_0$  is the value of this ratio at the reference pressure  $P_0$  or volume  $V_0$  and q a material-dependent parameter [7]. For sufficiently small volume changes we get  $q(1-\alpha_V)/\alpha_V=(1-\alpha_J)$  where  $\alpha_J=\frac{(J/W)_c}{(J/W)_0}$  and  $(J/W)_c=j(V_c)$ . This allows us to write

$$\Omega_V = \frac{\Gamma_V}{\kappa_0} = \frac{-xq}{1 - \alpha_J} \tag{6}$$

where the parameter q, which relates changes in volume to changes in the interactions, depends on the particular system. Taking q=5, for  $CeRu_2Si_2$  [7] and  $\nu z=1$ , as before, we get an enhancement for the thermal mass of approximately 36 for this system. In this way taking different values of q for different systems we may explain the hierarchy of thermal masses using the same critical exponents. Note that for  $CeAl_3$  the reference pressure  $P_0=1.2$ kbars such that  $m_T$  for this pressure is already very much reduced.

Let us return now to discuss the scaling relations obtained from the data of Figure 1, namely,  $2-\alpha=\nu z$  and  $\phi_h=\nu z$ . It is easy to verify that these equations imply a simple one-parameter scaling such that  $\chi_0^{-1} \propto m_T^{-1} \propto h_c \propto A^{-1/2} \propto T_{coh}$ , where A is the coefficient of the  $T^2$  term of the resistivity. As concerns the relations among the thermodynamic quantities they arise from a free energy obeying the simple scaling form,  $f \propto |\delta|^{\nu z} F[T/|\delta|^{\nu z}, h/|\delta|^{\nu z}]$ . This one-parameter scaling is reminiscent of single impurity and other phenomenological, non-critical, approaches to the heavy fermion problem [6]. In the former case the characteristic temperature is identified with the Kondo temperature. There

is however a fundamental difference between these approaches and the present scaling theory. Here the characteristic energy scale given by the coherence temperature  $T_{coh} \propto |(J/W) - (J/W)_c|^{\nu z}$  vanishes at the critical point of the Kondo lattice. Furthermore the scaling behavior found in these heavy fermion systems is due in our approach to their proximity to the QCP at  $(J/W) = (J/W)_c, T = 0, H = 0, h = 0$ . The vanishing of  $T_{coh}$  at the QCP led to the prediction [8] and observation of non-Fermi liquid behavior in heavy fermion systems [9].

The observation of one-parameter scaling in a three dimensional (d=3) critical theory with three independent exponents is clearly associated here with the breakdown of the hyperscaling relation  $2-\alpha=\nu(d+z)$ . Note that the relation  $2-\alpha=\nu z$  arising from the experimental data is the hyperscaling relation for d=0. It is not surprising then, that it yields scaling properties which are formally similar to those of a single impurity problem. Violation of hyperscaling is not uncommon in critical phenomena [4] and below we shall discuss the possible reasons it occurs here.

One-parameter scaling can also result from the constraints imposed by the Fermi liquid (FL) behavior below the coherence temperature. Let us assume that the entropy of the local moments, of total angular momentum J, for  $T >> T_{coh}$ ,  $S(T >> T_{coh}) = Nk_B Ln(2J+1)$  goes into that of the Fermi liquid which develops below  $T_{coh}$  and is given by,  $S(T \ll T_{coh}) = \int_0^{T_{coh}} dTC(T)/T$  with  $C(T) = m_T T$ . Equating both entropies we find  $m_T^{-1} \propto T_{coh}$ , which in turn implies  $2 - \alpha = \nu z$ . This argument [10] relies on the existence of a single characteristic temperature in the non-critical side of the phase diagram which is not necessarily always the case, as will be seen below [11].

### III. MICROSCOPIC MODEL

We now discuss a model of nearly antiferromagnetic Fermi liquid [12] which describes the results of the pressure experiments analyzed above. We start with the expression for the singular part of the free energy density of a nearly antiferromagnetic Fermi liquid due to spin fluctuations [13] [14] [15]:

$$f = -\frac{1}{\pi} \sum_{q} \int_{0}^{\infty} d\omega \coth(\beta \omega/2) \tan^{-1} \left[ \frac{I \Im m \chi^{0}(q,\omega)}{1 - I \Re e \chi^{0}(q,\omega)} \right]$$
(7)

where

$$\chi^0(Q+q,\omega) = \chi_Q(1 - aq^2 - b\omega^2 + ic\omega) \tag{8}$$

for  $q \ll Q$  and  $\omega \ll 1$ . At zero temperature we get

$$f = -\frac{1}{\pi} \sum_{q} \int_{0}^{\infty} d\omega \tan^{-1} \left[ \frac{I \chi_{Q} c\omega}{1 - I \chi_{Q} (1 - aq^{2} - b\omega^{2})} \right]$$

$$(9)$$

This can be rewritten as

$$f = -\frac{1}{\pi} \int d\vec{q} \int d\omega \tan^{-1} \left[ \frac{\omega \xi^z}{1 + q^2 \xi^2 + |\delta| (\omega \xi^z)^2} \right]$$
(10)

where the correlation length  $\xi = |\delta|^{-\nu}$  and the distance to the QCP,  $\delta = 1 - I\chi_Q$ . The correlation length exponent assumes the mean-field (or Gaussian) value,  $\nu = 1/2$  and the dynamic exponent, z = 2, typical of antiferromagnetic spin fluctuations. All constants have been taken equal to 1. In the limit  $\delta \to 0$ , a change of variable yields the scaling properties of this model. We find  $f \propto |\delta|^{\nu(d+z)}$ , where d is the dimension of the system, with additional scaling corrections due to the term  $|\delta|(\omega\xi^z)^2$ . From Eq.1, with F[0,0,0] = constant we obtain the generalized hyperscaling relation,  $2-\alpha = \nu(d+z)$  [2].

Let us consider the case of localized spin fluctuations [12], i.e., we neglect the q-dependence of  $\chi^0(q,\omega)$ . We get

$$f \propto \frac{1}{\pi} \int d\omega \tan^{-1} \left[ \frac{\omega \xi^z}{1 + |\delta|(\omega \xi^z)^2} \right]$$
 (11)

Now for  $\delta \to 0$ , we find  $f \propto |\delta|^{\nu z}$ , with scaling corrections. In this case, from Eq.1, we obtain  $2 - \alpha = \nu z$  and hyperscaling is violated due to the neglect of the q-dependence of  $\chi^0$ . Note that in this local theory the exponent  $\nu z = 1$  as for the nearly antiferromagnetic Fermi liquid.

For  $T \neq 0$  the relevant expression of the singular part of the free energy density is given by

$$f \propto -T \int^{q_c} d\vec{q} \int^{x_c} dx \coth x \tan^{-1} [xT\xi^z(1-$$

$$\frac{q^2\xi^2}{1+q^2\xi^2})]\tag{12}$$

which can be written in the form

$$f \propto |\delta|^{\nu(d+z)} F[T/T_{coh}]$$
 (13)

for  $x_c = \beta \omega_c/2 = 1/2$  and  $q_c \xi$  very large, as close to the critical point.

Again neglecting the q-dependent contribution we obtain, from Eq.12, the thermodynamic properties of the localized model. For  $xT\xi^z\ll 1$ , i.e.,  $\omega_c\xi^z\ll 1$  we may write  $\tan^{-1}y\approx y$ . Furthermore we take  $\hbar\omega_c=k_BT$ , in which case the constraint  $\omega_c\xi^z\ll 1$  implies  $T\ll T_{coh}\propto |\delta|^{\nu z}$ . In this regime the free energy exhibits Fermi liquid behavior and is given by,  $f\propto -(4/3)\pi q_c^3g(1/2)T^2\xi^z$ , where  $g(y)=\int_0^y dxx \coth x$ . The breakdown of the scale

invariant form, Eq.13 and consequently of hyperscaling is due to the neglect of the q-dependence. The thermal mass is given by

$$m_T^L = -\partial^2 f / \partial T^2 = m_M^0 (1/3) q_c^2 \xi^z \propto |\delta|^{-\nu z} = |\delta|^{-1}$$
 (14)

and diverges at the transition.  $m_M^0$  is a non-critical constant, which depends on local parameters and, linearly, on  $q_c$  [13].

Within the same Fermi liquid regime, for  $T \ll T_{coh}$ , the free energy given by Eq.12 can be calculated and the thermal mass is given by,  $m_T^M = -\partial^2 f/\partial T^2 = m_M^0 \left[1-(q_c\xi)^{-1}tan^{-1}(q_c\xi)\right]$ . In this case the thermal mass increases but does not diverge as the system approaches the critical point [13]. The second term in this expression for  $m_T^M$  is the universal scaling contribution, i.e., independent of the cut-off for  $q_c\xi \to \infty$ . It is proportional to  $\xi^{-1} \propto |\delta|^{1/2}$  since  $m_M^0 \propto q_c$ .

The free energies in the Fermi liquid regime  $(T \ll T_{coh})$ 

The free energies in the Fermi liquid regime  $(T \ll T_{coh})$  as a function of the distance to the QCP, for the localized and nearly antiferromagnetic (NAF) models are shown in Fig.2. Notice that for  $q_c \xi < 1/2$ , they nearly coincide. This can be seen directly, expanding  $m_T^M$  to obtain,  $m_T^M(q_c \xi \ll 1) \approx m_M^0(1/3)q_c^2 \xi^2 = m_T^L$  (see Eq.14). Then, in this regime [16] the scaling properties of both models are the same and they yield similar results, for example, for the relative pressure variation of the thermal mass,  $m_T(P_0)/m_T(P)$ .

For the resistivity in the local approximation we find [17]

$$\rho = \frac{\rho_0}{T\xi^z} \int_0^\infty dx \frac{x^2}{(e^{\frac{x}{T\xi^z}} - 1)(1 - e^{-\frac{x}{T\xi^z}})(1 + x^2)}$$
 (15)

For  $T\xi^z \ll 1$ , i.e.,  $T \ll T_{coh} = \xi^{-z} = |\delta|^{\nu z}$ , we get,  $\rho(T \ll T_{coh}) = \rho_0(\pi^2/3)(T/T_{coh})^2$  and for higher temperatures  $\rho(T >> T_{coh}) = \rho_0(\pi/2)(T/T_{coh})$  [17].

As concerns the magnetic field the experimental relation  $\phi_h = \nu z$  implies that the characteristic field  $h_c \propto |\delta|^{\nu z}$ . In fact, in the local approach, the uniform magnetic field h simply adds to the frequency a precession term [18]. Then at T=0

$$f \propto \frac{1}{\pi} \int d\omega \tan^{-1} \left[ (\omega + h) \xi^z \right]$$
 (16)

and  $\chi_0(T=0) = \partial^2 f/\partial h^2 \propto |\delta|^{-\nu z}$  with  $\nu z=1$ . This yields a diverging or enhanced uniform susceptibility but this result ceases to be valid sufficiently close to the critical point  $(q_c \xi > 1)$ .

It is clear from the results above that the theory of antiferromagnetic local spin fluctuations, with a single characteristic energy scale,  $T_{coh} \propto |\delta|^{\nu z}$ , such that  $f(T=0) \propto |\delta|^{\nu z} = T_{coh}$ ,  $m_T \propto |\delta|^{-\nu z} = T_{coh}^{-1}$ ,  $\chi_0(T=0) \propto |\delta|^{-\nu z} = T_{coh}^{-1}$  and  $\rho(T \ll T_{coh}) = AT^2$  with  $A \propto T_{coh}^{-2}$  correctly describes the pressure experiments we analyzed before. Furthermore in this approach

the crossover exponent  $\nu z=1$ . This provided the motivation for assuming this value for  $\nu z$  in the calculation of the enhancement factors in Section II of this paper.

The theory of localized antiferromagnetic paramagnons can be summarized in the scaling form of the free energy,  $f \propto |\delta|^{\nu z} F[T/|\delta|^{\nu z}, h/|\delta|^{\nu z}]$  with  $\nu z = 1$ . Although this is in agreement with the pressure experiments in a region of the phase diagram, for  $(J/W) > (J/W)_c$ ,  $T \leq T_{coh}$ , as the systems get closer to the critical point and  $q_c \xi \to \infty$  the full q-dependence of the dynamic susceptibility must be taken into account. The local theory also does not describe the non-Fermi liquid behavior observed at  $(J/W) = (J/W)_c$ ,  $T \to 0$ . For example, it's result for the specific heat at  $|\delta| = 0$  is given by,  $C = (3/2)Nk_B$ , i.e., that of a classical gas of N free particles. Sufficiently close to the QCP it is then necessary to consider the q-dependence of  $\chi^0(Q+q,\omega)$ . Taking this into account we obtain the universal contribution for the free energy at the  $QCP,\ f[\delta=0] \propto T^{\frac{d+z}{z}},$  in agreement with Eq.13, and the specific heat  $C/T(\delta = 0) \propto$  $\partial^2 f / \partial T^2 \propto T^{1/2}$  for d = 3, z = 2 with  $\nu z = 1$  [14,19,15].

### IV. GENERALIZED SCALING

It is important to point out that the result  $C/T \propto T^{1/2}$  at  $|\delta| = 0$  which arises from the scaling form Eq.13 is valid only in the case of extended scaling, i.e.,  $\psi = \nu z$ . Here  $\psi$  is the shift exponent such that the Neel temperature,  $T_N \propto |\delta|^{\psi}$ , close to the QCP [11] (see Fig.3). It turns out, experimentally, that  $\psi = 1$  [9] however, theoretically, one gets,  $\psi = z/(d+z-2) = 2/3 \neq \nu z = 1$  [14,19,15]. In this case a more general scaling form for the free energy is required to describe the complex critical behavior in the neighborhood of the QCP [11]. It is given by [11],

$$f \propto |\delta(T)|^{2-\alpha} F_c[t]$$

$$t = \frac{T}{\left|\delta(T)\right|^{\nu z}}\tag{17}$$

with

$$\delta(T) = \delta(T=0) - T^{1/\psi}$$

The singularities along the Neel line,  $|\delta(T)| = 0$ , are described by a new set of tilde exponents  $\tilde{\alpha}$ ,  $\tilde{\nu}$ , etc., different from those associated with the zero temperature fixed point (the non-tilde exponents). The scaling function  $F_c[t=0] = constant$  and  $F_c[t\to\infty] \propto t^x$  with  $x=(\tilde{\alpha}-\alpha)/\nu z$  such that close to the critical Neel line we obtain the correct asymptotic behavior,  $f \propto A(T)|\delta(T)|^{2-\tilde{\alpha}}$ , where the amplitude  $A(T)=T^{\frac{\tilde{\alpha}-\alpha}{\nu z}}$ . It is easy to verify that in the case of extended scaling, i.e.,  $\psi=\nu z$ , the exponents associated with the zero temperature fixed point are sufficient to describe the behavior along the non-Fermi liquid trajectory,  $|\delta|=0$ ,  $T\to 0$ 

and one finds the previous result,  $C/T \propto T^{\frac{d-z}{z}}$ . However in the situation here, where  $\psi=2/3<\nu z=1$ , the *tilde* exponents also play a role in determining the behavior along this path, which is tangent to the Neel line at the quantum multicritical point as shown in Fig.3. We find for the specific heat

$$C/T \propto T^{\frac{(2-\tilde{\alpha})(\nu z - \psi) + \nu \psi(d-z)}{\nu z \psi}} \tag{18}$$

Assuming thermal Gaussian exponents, essentially  $\tilde{\alpha}=1/2$ , we get,  $C/T \propto T^{5/4}$  for  $\psi=2/3, \nu=1/2$  and z=2, instead of  $C/T \propto T^{1/2}$  for the case of extended scaling. The staggered susceptibility  $\chi_Q(\delta=0,T) \propto T^{-\tilde{\gamma}/\psi}=T^{-3/2}$  since  $\gamma=\tilde{\gamma}=1$  [13].

An interesting possibility has been raised by Rösch at al. [20] who claimed that two-dimensional fluctuations are those relevant to describe the observed critical behavior. In this case scaling is extended since  $\psi = z/(d+z-2) = \nu z = 1$ . This approach leads to  $C/T(\delta=0) \propto LnT$  at the QCP and in the Fermi liquid regime, for  $T \ll T_{coh}$ , to  $m_T \propto Ln|\delta|$ .

#### V. ABOVE THE UPPER CRITICAL DIMENSION

In quantum phase transitions the relevant dimensionality is  $d_{eff} = d + z$ , as is evident from the modified hyperscaling relation,  $2 - \alpha = \nu(d+z)$ . In the problems we have studied above, it turns out that  $d_{eff} > d_c$ , where,  $d_c = 4$  is the upper critical dimension for these magnetic transitions. This is the reason Gaussian theories, as the SCR theory of spin fluctuations [13], provide an adequate description of the quantum critical point in nearly ferro and antiferromagnetic 3d materials [19]. Let us consider further implications of the fact that  $d+z>d_c=4$ . Consider the expression for the singular part of the  $T\,=\,0$ free energy,  $f \propto |\delta|^{\nu(d+z)}$ . Since the Gaussian exponent  $\nu = 1/2$ , whenever d + z > 4, we can rewrite it as,  $f \propto |\delta|^{2-\alpha}$  with  $\alpha < 0$ . In this case an analytic expansion of the free energy close to the critical point, such that,  $f \propto |\delta|^2$ , will always dominate the Gaussian contribution for  $\delta$  sufficiently small. The total free energy, in the non-critical side of the phase diagram, below the coherence line, can be written as a sum of an analytic term and a Gaussian contribution,

$$f_t = |\delta|^2 + |\delta|^{\nu(d+z)} F\left[\frac{T}{|\delta|^{\nu z}}\right]$$
(19)

where we neglected the temperature dependence of the analytic part assuming it is less singular than that of the Gaussian. In the Fermi liquid regime, i.e.,  $T \ll T_{coh} = |\delta|^{\nu z}$ , we have [3],

$$f_t = |\delta|^2 + |\delta|^{\nu(d+z)} \left\{ 1 + \left( \frac{T}{|\delta|^{\nu z}} \right)^2 + \cdots \right\}$$
 (20)

then, sufficiently close to the critical point and for d+z > 4, with  $\nu = 1/2$ , we obtain,

$$f_t = |\delta|^2 + |\delta|^{\nu(d+z)} \left(\frac{T}{|\delta|^{\nu z}}\right)^2 + \cdots$$
 (21)

which can be rewritten in the scaling form

$$f_t = |\delta|^2 F\left[\frac{T}{T_{sf}}\right] \tag{22}$$

where the value of  $\alpha = 0$  in the equation above, see Eq.1, can be associated with the breakdown of hyperscaling for d+z>4. The new spin-fluctuation temperature is given by

$$T_{sf} = \left|\delta\right|^{1 - \frac{d - z}{4}} \tag{23}$$

where we used  $\nu=1/2$ . Consequently the effect of the analytic contribution is to introduce a new energy scale in the Fermi liquid region of the phase diagram [21], namely  $T_{sf}$ . If we calculate the specific heat from the above expression for the free energy, we get,  $C/T \propto |\delta|^{\nu(d-z)}$  which of course coincides with the Gaussian result. On the other hand taking into account the field dependence of the analytic (mean-field) and Gaussian contributions, it can be easily shown that the order parameter linear susceptibility,  $\chi_0 = \left(\partial^2 f/\partial h^2\right)_{h=0}$  with  $f \propto |\delta|^2 F_0(T/T_{sf}, h/|\delta|^{\beta+\gamma})$  is given by  $\chi_0 = |\delta|^{-1} F_1(T/T_{sf})$ , for  $T \ll T_{coh}$ , where we used the mean field exponents,  $\beta = 1/2$  and  $\gamma = 1$ . The field h here is that conjugated to the order parameter.

We point out also that, because d+z>4, even at  $|\delta|=0$  there is a characteristic field  $h_{cross}=J$  which yields the crossover from mean-field to Gaussian behavior [11]. J is the actual critical coupling between localized and itinerant electrons [4]. The order parameter m at the quantum critical point varies with the conjugated field h, according to  $m \propto (h/J)^{1/\delta}$  [4]. For small fields, i.e.,  $h \ll h_{cross}$ , the mean-field contribution with  $\delta_{MF}=3$  dominates while in the opposite case the Gaussian one with  $\delta_G=\frac{d+z+2}{d+z-2}$  [11] is dominant (in the situation of interest here d=3 and z=2 such that  $\delta_G=7/3<\delta_{MF}=3$ ).

Finally note that the above discussion does not affect the local spin fluctuation results since, in this case the T=0 free energy is more *singular* than the analytic contribution, at least for  $\nu z < 2$ .

### VI. CONCLUSIONS

Our analysis of the pressure dependence of several physical quantities for different heavy fermions on a region of the phase diagram, for  $(J/W) > (J/W)_c$ ,  $T \le T_{coh}$ , has shown that these systems are close to a quantum critical point and a scaling approach is indeed appropriate. We have obtained from the experimental data, Grüneisen parameters which yield the enhancement factors due to the proximity of the QCP. It turns out that

a one-parameter scaling is sufficient to describe the experiments in this region of the phase diagram and this is associated with the violation of the hyperscaling relation. This one-parameter scaling here is different from that of single impurity approaches where the characteristic energy scale is identified with the Kondo temperature. In our case  $T_{coh}$  vanishes at the quantum critical point and this leads to the appearance of non-Fermi liquid behavior at  $\delta = 0$ . We have shown that a theory of localized spin fluctuations, with  $\nu z = 1$ , describes the pressure experiments summarized in Fig.1. For these experiments the *q-dependence* of the dynamic susceptibility plays no role. Physically this must be related to the fact that the actual spectrum of spin fluctuations is nearly q-independent, at least in the relevant directions of q-space, in this part of the phase diagram. This region corresponds to the case  $q_c \xi < 1/2$  of the NAF model since, as we have shown, the scaling properties of this and the local model are the same in this regime. In fact the local approach can be obtained as an expansion of the full q-dependent theory of antiferromagnetic spin fluctuations for  $q_c \xi \ll 1$  (see also [16]). Then it holds in a region, not too close to the QCP, but where scaling, specific to this q-independent regime (one-parameter scaling), still applies. The local theory allows for an explicit calculation of the Wilson  $(m_T/\chi_0)$ and Kadowaki-Woods  $(A/m_T^2)$  ratios [8] which turn out to be constants, i.e., independent of the distance to the critical point.

As the system moves closer to the critical point  $(q_c\xi \to \infty)$  we leave the limit of validity of the local theory and the full q-dependent susceptibility must be used. In both cases  $\nu z=1$ . In the q-dependent regime a generalized scaling theory is required to describe the complex critical behavior in the neighborhood of the QCP since the *shift* and crossover exponents are different for nearly antiferromagnetic 3d systems. This is particularly relevant along the *non-Fermi liquid trajectory* which is tangent to the QCP for  $\psi=2/3<1$ . It turns out that the exponents along this line depend on the thermal exponents characterizing the singularities on the Neel line, besides those associated with the QCP.

Although for the systems investigated the effective dimension  $d+z>d_c$ , it is the local nature of the spin fluctuation spectrum in the part of the phase diagram investigated that is responsible for the breakdown of hyperscaling and one-parameter scaling, observed in the experiments. In the microscopic approach the violation of hyperscaling can be traced to the cut-off acting as a relevant variable.

The purpose of a scaling theory of heavy fermions is to provide a unified description, in terms of a set of critical exponents, not only of the non-Fermi liquid regime but also of both sides of the quantum critical point. While most of the studies have been carried on in the non-critical side we also expect to find scaling behavior on the ordered region of the phase diagram, i.e., for  $(J/W) < (J/W)_c$ , where the systems at T=0 have long range magnetic order. We hope future studies will also

include this interesting region and also a larger class of materials [22].

### ACKNOWLEDGMENTS

I would like to thank Sergey Budko and Claudine Lacroix for discussions and a critical reading of the manuscript. Also I thank the LEPES-CNRS and in particular J-L. Tholence for the hospitality in Grenoble, where part of this work was carried out.

### **APPENDIX:**

We discuss here the limit  $q_c \xi \ll 1$  in relation to the theory of Ref. [15]. The free energy is given by,

$$f = -\frac{3T}{\pi} \int_0^{q_c} d\vec{q} \int_0^{x_c} dx \coth x \tan^{-1} \left[ \frac{xT}{J_Q - J_Q^c + Aq^2} \right]$$
(24)

where  $x = \frac{\beta \omega}{2}$ .  $J_Q$  is the q-dependent exchange coupling between the local moments at the wavevector Q of the incipient magnetic instability and  $J_Q^c$  its critical value. A is the *stiffness* of the spin fluctuations defined by the small wavevector expansion of the magnetic coupling close to the wavevector Q, i.e.,  $J_Q - J_{Q+q} = Aq^2 + \cdots$ .

A redefinition of the relevant quantities yields,

$$f = -\frac{3T}{\pi} \int_0^{q_c} d\vec{q} \int_0^{x_c} dx \coth x \tan^{-1} \left[ \frac{xT\xi^z}{A(1+q^2\xi^2)} \right]$$
(25)

where the correlation length  $\xi$  may be written as,  $\xi = \alpha \xi_L$  with  $\alpha = (A/J_Q a^2)^{1/2}$ ,  $\xi_L = a|\delta|^{-1/2}$  and  $\delta = 1 - (J_Q^c/J_Q)$ , such that,  $\nu = 1/2$ . a is an interatomic distance and the dynamic exponent z=2. Since  $1/(1+y^2) \leq 1$ , for  $\frac{x_c T \xi^z}{A} \ll 1$ , or equivalently,  $\omega_c \xi_L^z \ll 1$ , which assuming  $\hbar \omega_c = k_B T$  implies  $T \ll T_{coh} \propto \xi_L^{-z}$ , we can expand the  $\tan^{-1}$  for small arguments. In this regime the free energy exhibits Fermi liquid behavior. Performing the integrations, we get

$$f \approx -\frac{12T^2\xi^{(z-d)}}{A}g(1/2)q_c\xi\left(1 - \frac{\tan^{-1}q_c\xi}{q_c\xi}\right)$$
 (26)

where  $g(y) = \int_0^y x \coth x dx$ . The limit  $q_c \xi \ll 1$  is obtained, either because the system is not too close to the QCP, i.e.,  $|\delta|$  is large, or  $A \to 0$  due to the localization of the fluctuations, we get

$$f \propto \frac{12T^2}{A}g(1/2)q_c \left[\frac{1}{3}(q_c\xi)^2 - \frac{1}{5}(q_c\xi)^4 + \cdots\right]$$
 (27)

Using  $\xi = \alpha \xi_L$ , as defined above, we get

$$f \approx -\frac{4T^2 \xi_L^2}{J_Q a^2} g(1/2) q_c^3 + \frac{12AT^2 \xi_L^4}{5J_Q^2 a^4} g(1/2) q_c^5 + O(A^2)$$
(28)

The first term is independent of A and corresponds to the localized model where the stiffness A vanishes. The validity of the local theory is then given by  $q_c \xi \ll 1$  or  $q_c \xi_L \ll (J_Q a^2/A)^{1/2}$  such that when  $A \to 0$  the local model becomes valid arbitrarily close to the QCP.

- [1]
- [2] M.A. Continentino, G. Japiassu and A. Troper, Phys. Rev. B39, 9734 (1989).
- [3] M.A. Continentino, Phys. Rev. **B47**, 11587 (1993).
- [4] M. A. Continentino, Physics Reports, Vol. 239, n. 3, 179 (1994) and references therein.
- [5] M.A. Continentino, Zeitschrift für Physik **B101**, 197 (1996).
- [6] see J.D. Thompson and J. M. Lawrence, in *Handbook on the Physics and Chemistry of Rare Earths*, Chapter 133, p. 383, Vol.19 Lanthanides/Actinides:Physics-II, edited by K.A. Gschneider Jr., L. Eyring, G.H. Lander and G.R. Choppin, Elsevier Science B.V., 1994.
- [7] M. Lavagna, C. Lacroix and M.Cyrot, Phys.Lett. 90A, 210 (1982).
- [8] M. A. Continentino, J. de Physique **I1**, 693 (1991).
- [9] H. v. Löhneysen et al., Phys.Rev.Lett.**72**, 3262 (1994).
- [10] Z. Fisk, Lecture notes, unpublished.
- [11] M.A. Continentino, Phys. Rev. **B55**, 5589 (1997).
- [12] C. Pinettes and C.Lacroix, J.Phys.:Condens.Matter, 6, 10093 (1994); C. Lacroix and C. Pinettes, Physica B 206&207, 11 (1995); S. Kambe et al., J.Phys.Soc.Japan, 65, 3294 (1996).
- [13] T. Moriya, in Spin Fluctuations in Itinerant Electron Magnetism, Springer-Verlag, Berlin Heidelberg, 1985.
- [14] H. Hasegawa, J. Phys. Soc. Jap. 38, 107 (1975).
- [15] T. Moriya and T. Takimoto, J. Phys. Soc. Jpn. 64, 960 (1995).
- [16] It is interesting to discuss the limit  $q_c \xi \ll 1$  in relation to the theory of Ref. [15], which is formally similar to the one presented here. In this approach the correlation length as appears in Eqs. 10 and 12 is given by,  $\xi = (A/|\delta|)^{1/2}$ , where A is the stiffness of the spin fluctuations. It is defined by  $J_Q J_{Q+q} = Aq^2 + \cdots$  with  $J_Q$  the q-dependent exchange coupling at the wavevector Q of the incipient instability. Then, in this approach, the limit  $q_c \xi \ll 1$  is obtained either because the system is not too close to the QCP, i.e.,  $|\delta|$  is large, or A is small due to the localization of the fluctuations. In this limit one recovers again from this theory the thermodynamic properties of the local model.
- [17] P. Lederer and D.L. Mills, Phys.Rev. 165, 837 (1968);
   A.B. Kaiser and S. Doniach, Intern. J. Magnetism 1, 11 (1970).

- [18] S. Sachdev, Z.Phys. **B94**, 469 (1994).
- [19] A.J. Millis, Phys. Rev. **B48**, 7183 (1993).
- [20] A. Rosch, A. Schröder, O. Stockert and H. v. Löhneysen, Phys.Rev.Lett. 79, 159 (1997).
- [21] M.T. Beal-Monod, S.K. Ma and D.R. Fradkin, Phys.Rev.Lett. 20, 929, (1968).
- [22] F. Steglich, C. Geibel, R. Modler, M. Lang, P. Hellmann and P. Gegenwart, J. Low Temp. Phys. 99, 267 (1995).

# TABLE

Compound	$\Gamma_V$	$\kappa_0$	$\Omega_V = \Gamma_V / \kappa_0$	$\alpha_V = V_0/V_c$
$CeAl_3$	89	2.17	41	0.976
$CeRu_2Si_2$	171	0.95	180	0.994
$UPt_3$	26	0.48	54	0.981
$CeCu_6$	133	1.1	121	0.992

TABLE I. Grüneisen parameters for different heavy fermions according to the relative pressure variation of several physical quantities shown in Fig. 1 [3].  $\Gamma_V$  and the compressibility  $\kappa_0$  are in  $Mbar^{-1}$ . The reference pressure for  $CeAl_3$  is  $P_0 = 1.2$  kbars otherwise  $P_0 = 0$ . The data for  $CeCu_6$  is taken from Ref. [6] and references therein.

## FIGURE CAPTIONS

Figure 1. Semi-logarithmic plot of  $X(P)/X(P_0)$  for several physical quantities, at or below  $T_{coh}$ , as a function of pressure for different heavy fermions [3]. For  $CeAl_3$ ,  $P_0 = 1.2$  kbars otherwise  $P_0 = 0$ . The numbers close to the lines are their inclinations,  $\Gamma_V$ , given in Table I (also see text).

Figure 2. The free energy in the Fermi liquid regime, at a fixed temperature  $T_0 \ll T_{coh}$ , for the localized and nearly antiferromagnetic models as a function of the distance to the critical point, located at  $(q_c \xi)^{-1} = 0$ . For  $(q_c \xi)^{-1} > 2$  the free energies of both models nearly coincide and consequently have the same scaling behavior.

Figure 3. Phase diagram of a nearly antiferromagnetic 3d system, with the shift exponent  $\psi=2/3$  and the crossover exponent  $\nu z=1$ . The tilde (thermal) exponents determine the critical behavior on the Neel line. In this case of  $\psi<1$ , the non-Fermi liquid trajectory is tangent to the quantum critical point and the thermal exponents besides those associated with the QCP are required to characterize the physical behavior along this line  $(|\delta|=0,T\to0)$ .





